

# Modern Energy Density Functional for Properties of Nuclei And The Current Status of The Equation of State of Nuclear Matter

Shalom Shlomo  
Texas A&M University

# Outline

## 1. Introduction.

Collective States, Equation of State,

## 2. Energy Density Functional.

Hartree-Fock Equations (HF), Skyrme Interaction

Simulated Annealing Method, Data and Constraint

## 3. Results and Discussion.

## 4. HF-based Random-Phase-Approximation (RPA).

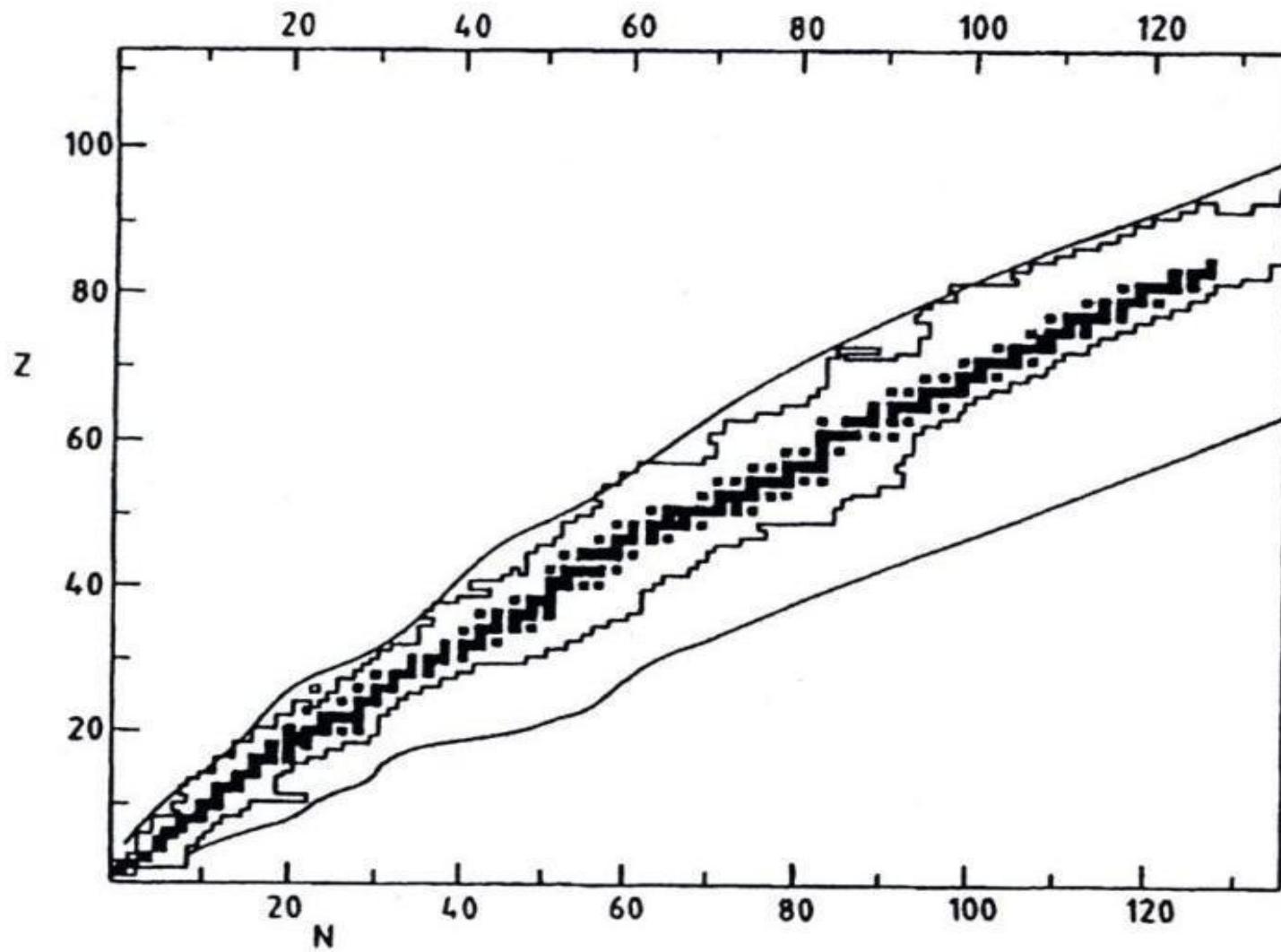
Fully Self Consistent HF-RPA, Compression Modes and the  
NM EOS, Symmetry Energy Density

## 5. Results and Discussion.

## 6. Conclusions.

# Introduction

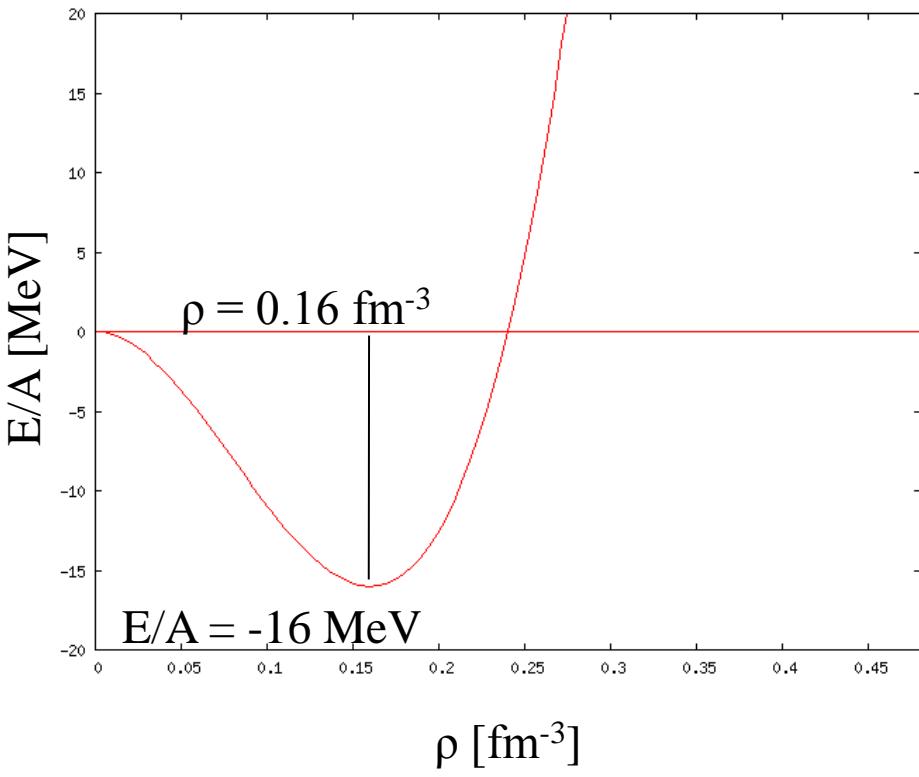
1. Important task: Develop a modern Energy Density Functional (EDF),  $E = E[\rho]$ , with enhanced predictive power for properties of rare nuclei.
2. We start from EDF obtained from the Skyrme N-N interaction.
3. The effective Skyrme interaction has been used in mean-field models for several decades. Many different parameterizations of the interaction have been realized to better reproduce nuclear masses, radii, and various other data. Today, there is more experimental data of nuclei far from the stability line. It is time to improve the parameters of Skyrme interactions. We fit our mean-field results to an extensive set of experimental data and obtain the parameters of the Skyrme type effective interaction for nuclei at and far from the stability line.



Map of the existing nuclei. The black squares in the central zone are stable nuclei, the broken inner lines show the status of known unstable nuclei as of 1986 and the outer lines are the assessed proton and neutron drip lines (Hansen 1991).

# Equation of state and nuclear matter compressibility

The symmetric nuclear matter ( $N=Z$  and no Coulomb) incompressibility coefficient,  $K$ , is an important physical quantity in the study of nuclei, supernova collapse, neutron stars, and heavy-ion collisions, since it is directly related to the curvature of the nuclear matter (NM) equation of state (EOS),  $E = E(\rho)$ .



$$E_{ANM}[\rho_o(\beta)] = E[\rho_o(\beta)] + \frac{1}{18} K(\rho_o(\beta)) \left( \frac{\rho - \rho_o(\beta)}{\rho_o(\beta)} \right)^2$$

$$E[\rho_o(\beta)] = E[\rho_o] + J\beta^2$$

$$K[\rho_o(\beta)] = K + K_\pi \beta^2$$

$$E_{SYM}(\rho) = \frac{1}{8} \left. \frac{d^2(E/A)}{dy^2} \right|_{\rho, y=1/2}$$

$$J = E_{SYM}[\rho_o]$$

$$\beta = (N - Z)/A \qquad \qquad y = Z/A$$

# Modern Energy Density Functional

The total Hamiltonian of the nucleus

$$\hat{H}_{total} = \sum_i \left[ -\frac{\hbar^2}{2m} \nabla_{r_i}^2 + V_{i,i}^{NN} + V_{i,i}^{GC} \right]$$

where

$$V_{i,j}^{GC} = V_{ij}^{NN} + V_{ij}^{GC}.$$

HF equations: minimize

$$E \langle \Phi | \hat{H}_{total} | \Phi \rangle$$

Within the HF approximation: the ground state wave function  $\Phi$

# Skyrme interaction

For the nucleon-nucleon interaction

$$\vec{V}_{ij} = V_{ij}^{NN} V_{ij}^{Gc}.$$

$$V_{ij}^{Gout} = \frac{2}{4} \frac{\tau_i + \tau_j}{\tau_i - \tau_j}, \quad \tau_{ij} = \tau_i + \tau_j$$

$V_{ij}^{NN}$  we adopt the standard Skyrme type interaction

$$\begin{aligned} V_{ij}^{NN} &= \frac{1}{2} \left( \alpha_{ij} \vec{P}_i \cdot \vec{Q}_j + \frac{1}{2} \alpha_{ij} \vec{Y}_{ij} \cdot \vec{M}_j \right) + \frac{1}{2} \left( \alpha_{ij} \vec{P}_j \cdot \vec{Q}_i + \frac{1}{2} \alpha_{ij} \vec{Y}_{ij} \cdot \vec{M}_i \right) \\ &+ \frac{1}{6} \left( \alpha_{ij} \vec{P}_i \cdot \vec{Q}_j + \frac{1}{2} \alpha_{ij} \vec{Y}_{ij} \cdot \vec{M}_j \right) \boxed{\frac{R_i R_j}{2}} + \dots \\ i \vec{W}_i &\vec{P}_i \cdot \vec{Q}_j \end{aligned}$$

$t_i, x_i, \alpha, W$  are 10 Skyrme parameters.

# The total energy

$$E = \langle \Phi | \hat{H}_{total} | \Phi \rangle = \langle \Phi | T + V_{Coulomb} + V_{12} | \Phi \rangle = \int H(\vec{r}) d\vec{r}$$

where

$$H(\vec{r}) = H_{Kinetic}(\vec{r}) + H_{Coulomb}(\vec{r}) + H_{Skyrme}(\vec{r})$$

$$H_{Kinetic}(\vec{r}) = \frac{\hbar^2}{2m_p} \tau_p(\vec{r}) + \frac{\hbar^2}{2m_n} \tau_n(\vec{r})$$

$$H_{Coulomb}(\vec{r}) = \frac{e^2}{2} \left[ \rho_{ch}(\vec{r}) \int \frac{\rho_{ch}(\vec{r}')}{|\vec{r} - \vec{r}'|} d\vec{r}' - \int \frac{|\rho_{ch}(\vec{r}, \vec{r}')|^2}{|\vec{r} - \vec{r}'|} d\vec{r}' \right]$$

$$H_{Skyrme}(\vec{r}) = H_0 + H_3 + H_{eff} + H_{fin} + H_{so} + H_{sg}$$

$$\mathcal{H}_0=\frac{1}{4}t_0\left[(2+x_0)\rho^2-(2x_0+1)(\rho_p^2+\rho_n^2)\right],$$

$$\mathcal{H}_3=\frac{1}{24}t_3\rho^\alpha\left[(2+x_3)\rho^2-(2x_3+1)(\rho_p^2+\rho_n^2)\right],$$

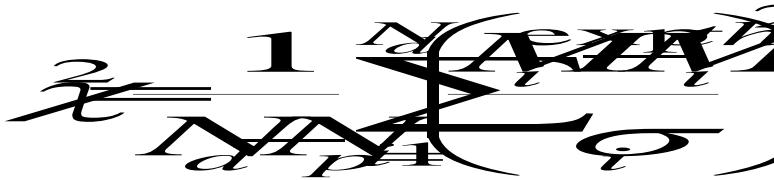
$$\mathcal{H}_{\text{eff}}=\frac{1}{8}\left[t_1(2+x_1)+t_2(2+x_2)\right]\tau\rho+\frac{1}{8}\left[t_2(2x_2+1)-t_1(2x_1+1)\right](\tau_p\rho_p+\tau_n\rho_n),$$

$$\begin{aligned}\mathcal{H}_{\text{fin}} &= \frac{1}{32}\left[3t_1(2+x_1)-t_2(2+x_2)\right](\nabla\rho)^2 \\&\quad -\frac{1}{32}\left[3t_1(2x_1+1)+t_2(2x_2+1)\right]\left[(\overrightarrow{\nabla}\rho_p)^2+(\overrightarrow{\nabla}\rho_n)^2\right],\\\mathcal{H}_{\text{so}} &= \frac{W_0}{2}\left[\mathbf{J}\cdot\nabla\rho+\mathbf{J}_p\cdot\nabla\rho_p+\mathbf{J}_n\cdot\nabla\rho_n\right],\\\mathcal{H}_{\text{sg}} &= -\frac{1}{16}(t_1x_1+t_2x_2)\mathbf{J}^2+\frac{1}{16}(t_1-t_2)\left[\mathbf{J}_p^2+\mathbf{J}_n^2\right].\end{aligned}$$

# Simulated Annealing Method (SAM)

The SAM is a method for optimization problems of large scale, in particular, where a desired global extremum is hidden among many local extrema.

We use the SAM to determine the values of the Skyrme parameters by searching the global minimum for the chi-square function



$N_d$  is the number of experimental data points.

$N_p$  is the number of parameters to be fitted.

$M_i^{\text{exp}}$  and  $M_i^{\text{th}}$  are the experimental and the corresponding theoretical values of the physical quantities.

$\sigma_i$  is the adopted uncertainty.

Implementing the SAM to search the global minimum of  $\chi^2$  function:

1.  $t_i, x_i, \alpha, W$  are written in term of  $B_A K_{nm} \rho_{nm}$
2. Define ~~the total energy~~
3. Calculate  $\chi^2_{old}$  for a given set of experimental data and the corresponding HF results (using an initial guess for Skyrme parameters).
4. Determine a new set of Skyrme parameters by the following steps:
  - + Use a random number to select a component  $v_r$  of vector  $\vec{v}$
  - + Use another random number  $\eta$  to get a new value of  $v_r$
$$v_r \rightarrow v_r + dr$$
  - + Use this modified vector  $\vec{v}$  to generate a new set of Skyrme parameters.

5. Go back to HF and calculate  $\chi^2_{new}$
6. The new set of Skyrme parameters is accepted only if



7. Starting with an initial value of  $T = T_i$ , we repeat steps 4 - 6 for a large number of loops.
8. Reduce the parameter T as  $T = \frac{T_i}{k}$  and repeat steps 1 – 7.
9. Repeat this until hopefully reaching global minimum of  $\chi^2$

# Fitted data

- The binding energies for 14 nuclei ranging from normal to the exotic (proton or neutron) ones:  $^{16}\text{O}$ ,  $^{24}\text{O}$ ,  $^{34}\text{Si}$ ,  $^{40}\text{Ca}$ ,  $^{48}\text{Ca}$ ,  $^{48}\text{Ni}$ ,  $^{56}\text{Ni}$ ,  $^{68}\text{Ni}$ ,  $^{78}\text{Ni}$ ,  $^{88}\text{Sr}$ ,  $^{90}\text{Zr}$ ,  $^{100}\text{Sn}$ ,  $^{132}\text{Sn}$ , and  $^{208}\text{Pb}$ .
- Charge rms radii for 7 nuclei:  $^{16}\text{O}$ ,  $^{40}\text{Ca}$ ,  $^{48}\text{Ca}$ ,  $^{56}\text{Ni}$ ,  $^{88}\text{Sr}$ ,  $^{90}\text{Zr}$ ,  $^{208}\text{Pb}$ .
- **The spin-orbit splittings for  $2p$  proton and neutron orbits for  $^{56}\text{Ni}$**   
 $\epsilon(2p_{1/2}) - \epsilon(2p_{3/2}) = 1.88 \text{ MeV (neutron)}$   
 $\epsilon(2p_{1/2}) - \epsilon(2p_{3/2}) = 1.83 \text{ MeV (proton)}.$
- **Rms radii for the valence neutron:**  
in the  $1d_{5/2}$  orbit for  $^{17}\text{O}$        $r_n(d_{5/2}) = 33.6$   
in the  $1f_{7/2}$  orbit for  $^{41}\text{Ca}$        $r_n(f_{7/2}) = 39.8$
- The breathing mode energy for 4 nuclei:  $^{90}\text{Zr}$  (17.81 MeV),  $^{116}\text{Sn}$  (15.9 MeV),  $^{144}\text{Sm}$  (15.25 MeV), and  $^{208}\text{Pb}$  (14.18 MeV).

# Constraints

1. The critical density

$$2\beta < \rho_{cr} < 3\epsilon$$



Landau stability condition:

$$E_i \dot{Q}_i - Q_i \dot{E}_i > 0$$

Example:

$$\frac{\partial}{\partial t} \left( \frac{P}{2m} \dot{Q}_i \right) > 0$$

2. The Landau parameter  $G_0'$  should be positive at  $\rho = \rho_0$

3. The quantity  $P = 3\rho \frac{dS}{d\rho}$  must be positive for densities up to  $3\rho_0$

4. The IVGDR enhancement factor  $0.25 < \kappa < 0.6$



	v	v <sub>0</sub>	v <sub>1</sub>	d
B/A (MeV)	16.0	17.0	15.0	0.4
K <sub>nm</sub> (MeV)	230.0	200.0	300.0	20.0
$\rho_{\text{nm}}$ (fm <sup>-3</sup> )	0.160	0.150	0.170	0.005
m*/m	0.70	0.60	0.90	0.04
E <sub>s</sub> (MeV)	18.0	17.0	19.0	0.3
J (MeV)	32.0	25.0	40.0	4.0
L (MeV)	47.0	20.0	80.0	10.0
Kappa	0.25	0.1	0.5	0.1
G'₀	0.08	0.00	0.40	0.10
W <sub>0</sub> (MeV fm <sup>5</sup> )	120.0	100.0	150.0	5.0

Values of the Skyrme parameters and the corresponding physical quantities of nuclear matter for the KDE0 and KDE0v1 and KDEX interactions.

Parameter	KDE0	KDE0v1	KDEX
$t_0$ (MeV fm <sup>3</sup> )	-2526.5110	-2553.0843	-1419.8304
$t_1$ (MeV fm <sup>5</sup> )	430.9418	411.6963	309.1373
$t_2$ (MeV fm <sup>5</sup> )	-398.3775	-419.8712	-172.9562
$t_3$ (MeV fm <sup>3(1+α)</sup> )	14235.5193	14603.6069	10465.3523
$x_0$	0.7583	0.6483	0.1474
$x_1$	-0.3087	-0.3472	-0.0853
$x_2$	-0.9495	-0.9268	-0.6144
$x_3$	1.1445	0.9475	0.0220
$W_0$ (MeV fm <sup>5</sup> )	128.9649	124.4100	98.8973
$\alpha$	0.1676	0.1673	0.4989
$B/A$ (MeV)	16.11	16.23	15.96
$K$ (MeV)	228.82	227.54	274.20
$\rho_0$ (fm <sup>-3</sup> )	0.161	0.165	0.155
$m^*/m$	0.72	0.74	0.81
$J$ (MeV)	33.00	34.58	32.76
$L$ (MeV)	45.22	54.69	63.70
$\kappa$	0.30	0.23	0.33
$G'_0$	0.05	0.00	0.41

# History

## A. ISOSCALAR GIANT MONOPOLE RESONANCE (ISGMR):

1977 – DISCOVERY OF THE CENTROID ENERGY OF THE ISGMR IN  $^{208}\text{Pb}$

$$E_0 \sim 13.5 \text{ MeV (TAMU)}$$

- This led to modification of commonly used effective nucleon-nucleon interactions. Hartree-Fock (HF) plus Random Phase Approximation (RPA) calculations, with effective interactions (Skyrme and others) which reproduce data on masses, radii and the ISGMR energies have:

$$K_\infty = 210 \pm 20 \text{ MeV (J.P. BLAIZOT, 1980).}$$

## A. ISOSCALAR GIANT DIPOLE RESONANCE (ISGDR):

1980 – EXPERIMENTAL CENTROID ENERGY IN  $^{208}\text{Pb}$  AT

$$E_1 \sim 21.3 \text{ MeV (Jülich), PRL 45 (1980) 337; } \sim 19 \text{ MeV, PRC 63 (2001) 031301}$$

- HF-RPA with interactions reproducing  $E_0$  predicted  $E_1 \sim 25 \text{ MeV}$ .

$$K_\infty \sim 170 \text{ MeV from ISGDR ?}$$

T.S. Dimitrescu and F.E. Serr [PRC 27 (1983) 211] pointed out “If further measurement confirm the value of 21.3 MeV for this mode, the discrepancy may be significant”.

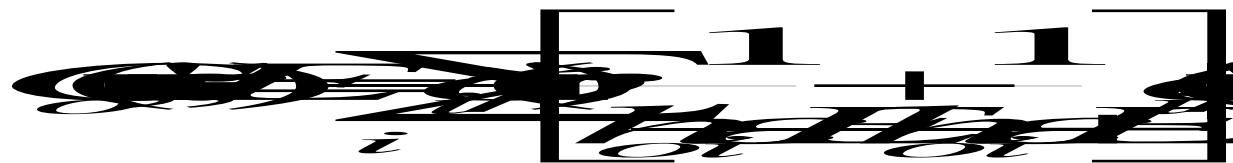
→ Relativistic mean field (RMF) plus RPA with NL3 interaction predict  $K_\infty=270 \text{ MeV}$  from the ISGMR [N. Van Giai et al., NPA 687 (2001) 449].

## Green's Function Formulation of RPA

In the Green's Function formulation of RPA, one starts with the RPA-Green's function which is given by

$$G(\epsilon) = G_0(\epsilon) + V_{ph} G_0^{-1}$$

where  $V_{ph}$  is the particle-hole interaction and the free particle-hole Green's function is defined as



where  $\phi_i$  is the single-particle wave function,  $\epsilon_i$  is the single-particle energy, and  $h_o$  is the single-particle Hamiltonian.

The continuum effects, such as particle escape width, can be taken into account using

$$\left\langle r_1 \left| \frac{1}{h_0 - Z} \right| r_2 \right\rangle = \frac{2m}{\hbar^2} U(r_<)V(r_>)/W$$

where  $r_<$  and  $r_>$  are the lesser and greater of  $r_1$  and  $r_2$  respectively, U and V are the regular and irregular solution of  $(H_0 - Z)\psi = 0$ , with the appropriate boundary conditions, and W is the Wronskian.

NOTE the two terms in the free particle-hole greens function

We use the scattering operator  $F$

$$F = \sum_{i=1}^A f(\mathbf{r}_i)$$

to obtain the strength function



and the transition density



$\delta\rho^{RPA}$  is consistent with the strength in  $E \pm \Delta E/2$



# Relativistic Mean Field + Random Phase Approximation

The steps involved in the relativistic mean field based RPA calculations are analogous to those for the non-relativistic HF-RPA approach. The nucleon-nucleon interaction is generated through the exchange of various effective mesons. An effective Lagrangian which represents a system of interacting nucleons looks like

$$\begin{aligned}\mathcal{L} = & \overline{\Psi} \left( i\gamma^\mu \partial_\mu - M_N - g_\sigma \sigma - g_\omega \gamma^\mu \omega_\mu - g_\rho \tau^a \gamma^\mu \rho_\mu^a - e \gamma^\mu A_\mu \frac{1}{2}(1 - \tau_3) \right) \Psi \\ & + \frac{1}{2} \partial^\mu \sigma \partial_\mu \sigma - U_\sigma - \frac{1}{4} W^{\mu\nu} W_{\mu\nu} + U_\omega + \frac{1}{2} m_\rho^2 \rho^{\alpha\mu} \rho_\mu^\alpha - \frac{1}{4} R^{\alpha\mu\nu} R_{\mu\nu}^\alpha \\ & - \frac{1}{4} F^{\mu\nu} F_{\mu\nu},\end{aligned}$$

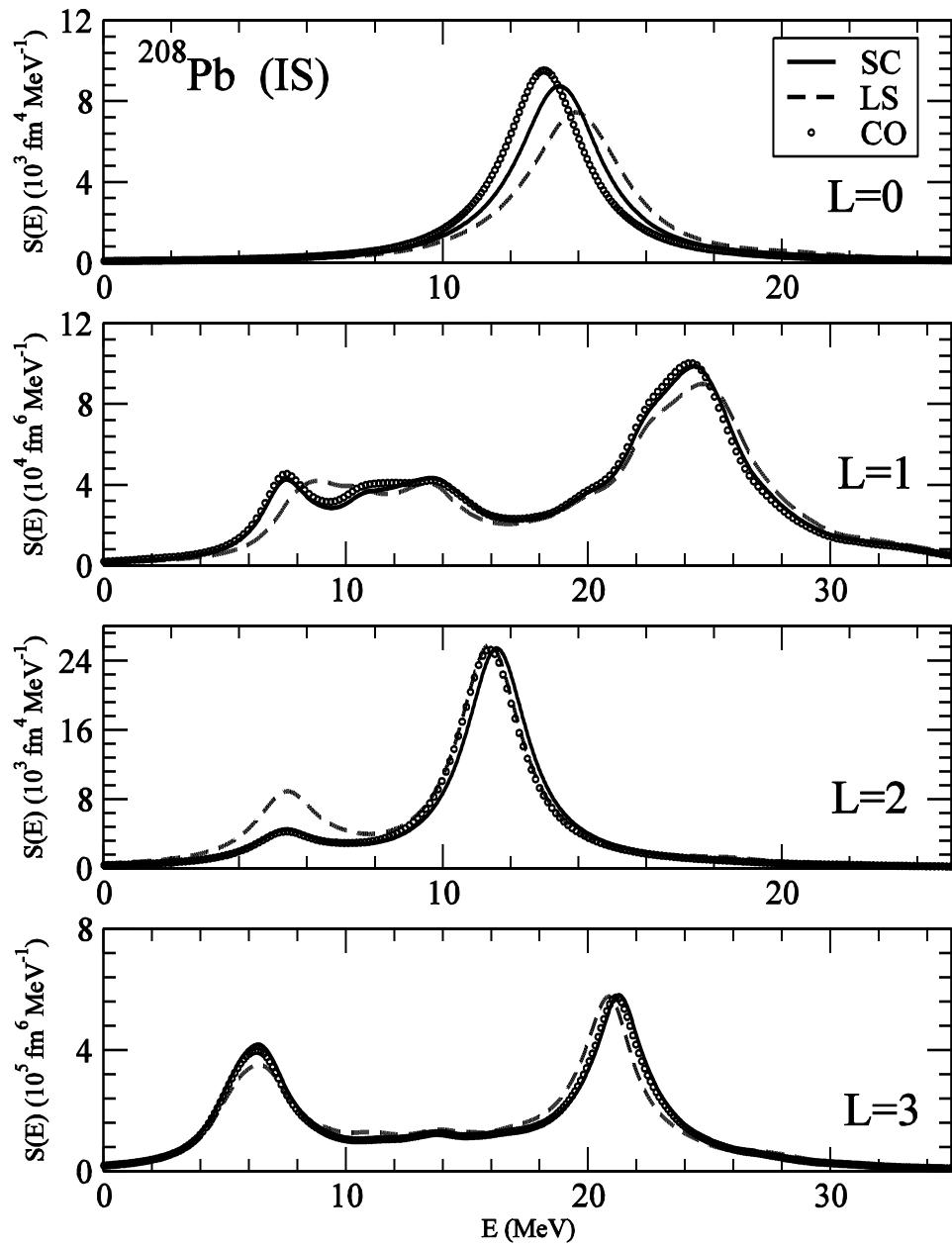
$$U_\sigma = \frac{1}{2} m_\sigma^2 \sigma^2 + \frac{1}{3} g_2 \sigma^3 + \frac{1}{4} g_3 \sigma^4, \quad U_\omega = \frac{1}{2} m_\omega^2 \omega^\mu \omega_\mu + \frac{1}{4} c_3 (\omega^\mu \omega_\mu)^2.$$

It contains nucleons ( $\psi$ ) with mass  $M$ ;  $\sigma$ ,  $\omega$ ,  $\rho$  mesons; the electromagnetic field; non linear self-interactions for the  $\sigma$  (and possibly  $\omega$ ) field.

Values of the parameters for the most widely used NL3 interaction are  $m_\sigma=508.194$  MeV,  $m_\omega=782.501$  MeV,  $m_\rho=763.000$  MeV,  $g_\sigma=10.217$ ,  $g_\omega=12.868$ ,  $g_\rho=4.474$ ,  $g_2=-10.431$  fm $^{-1}$  and  $g_3=-28.885$  (in this case there is no self-interaction for the  $\omega$  meson).

NL3:  $K_\infty=271.76$  MeV, G.A.Lalazissis et al., PRC 55 (1997) 540.

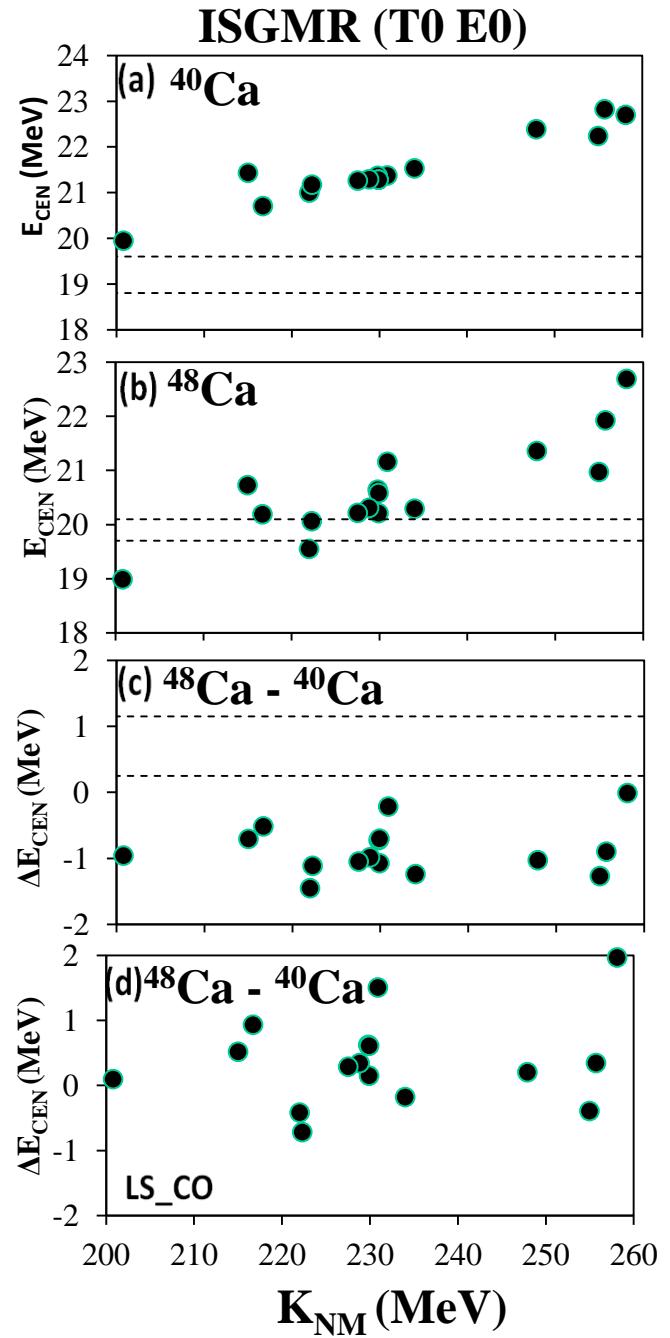
RMF-RPA: J. Piekarewicz PRC 62 (2000) 051304; Z.Y. Ma et al., NPA 686 (2001) 173.

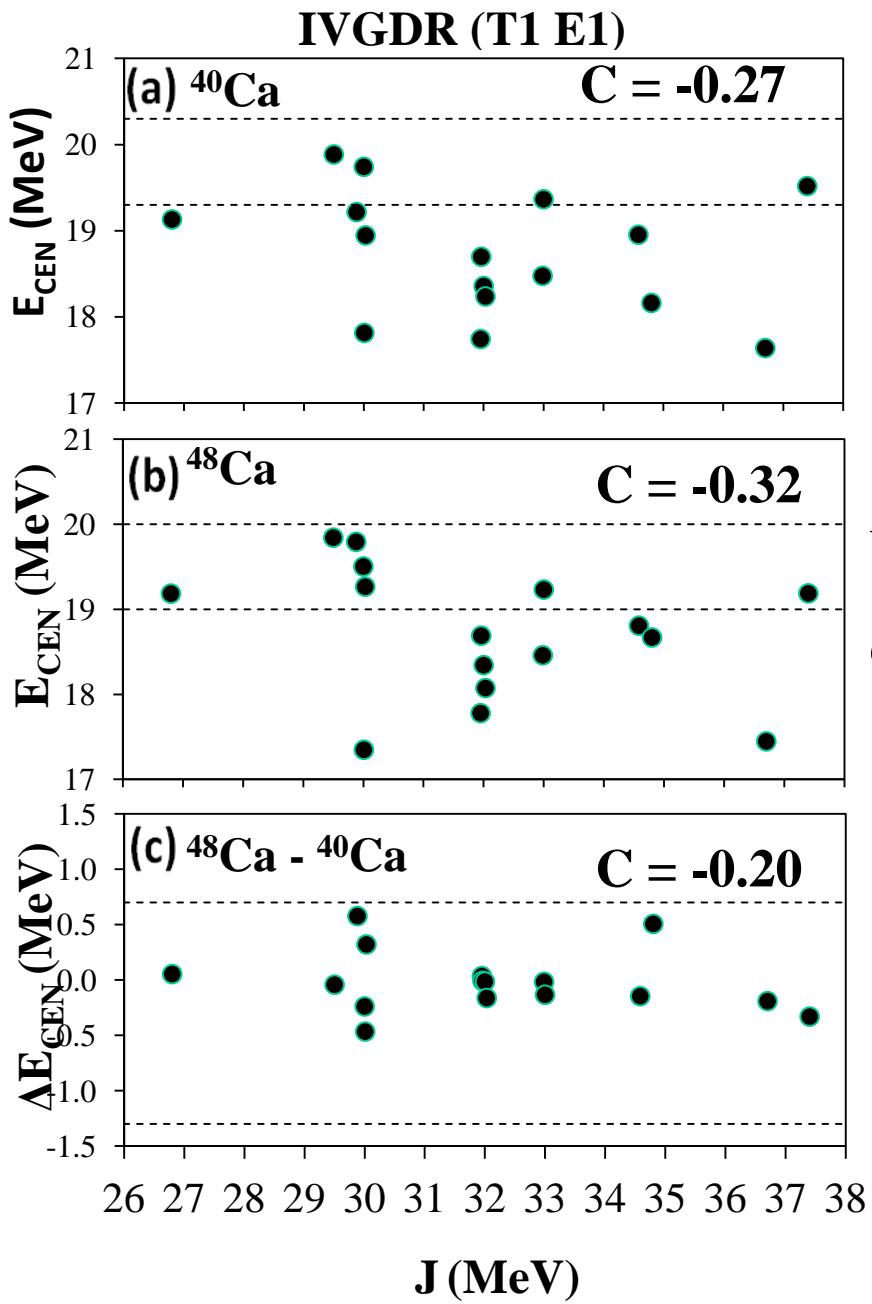


Isoscalar strength functions of  $^{208}\text{Pb}$  for  $L = 0 - 3$  multipolarities are displayed. The SC (full line) corresponds to the fully self-consistent calculation where LS (dashed line) and CO (open circle) represent the calculations without the ph spin-orbit and Coulomb interaction in the RPA, respectively. The Skyrme interaction SGII [Phys. Lett. B **106**, 379 (1981)] was used.

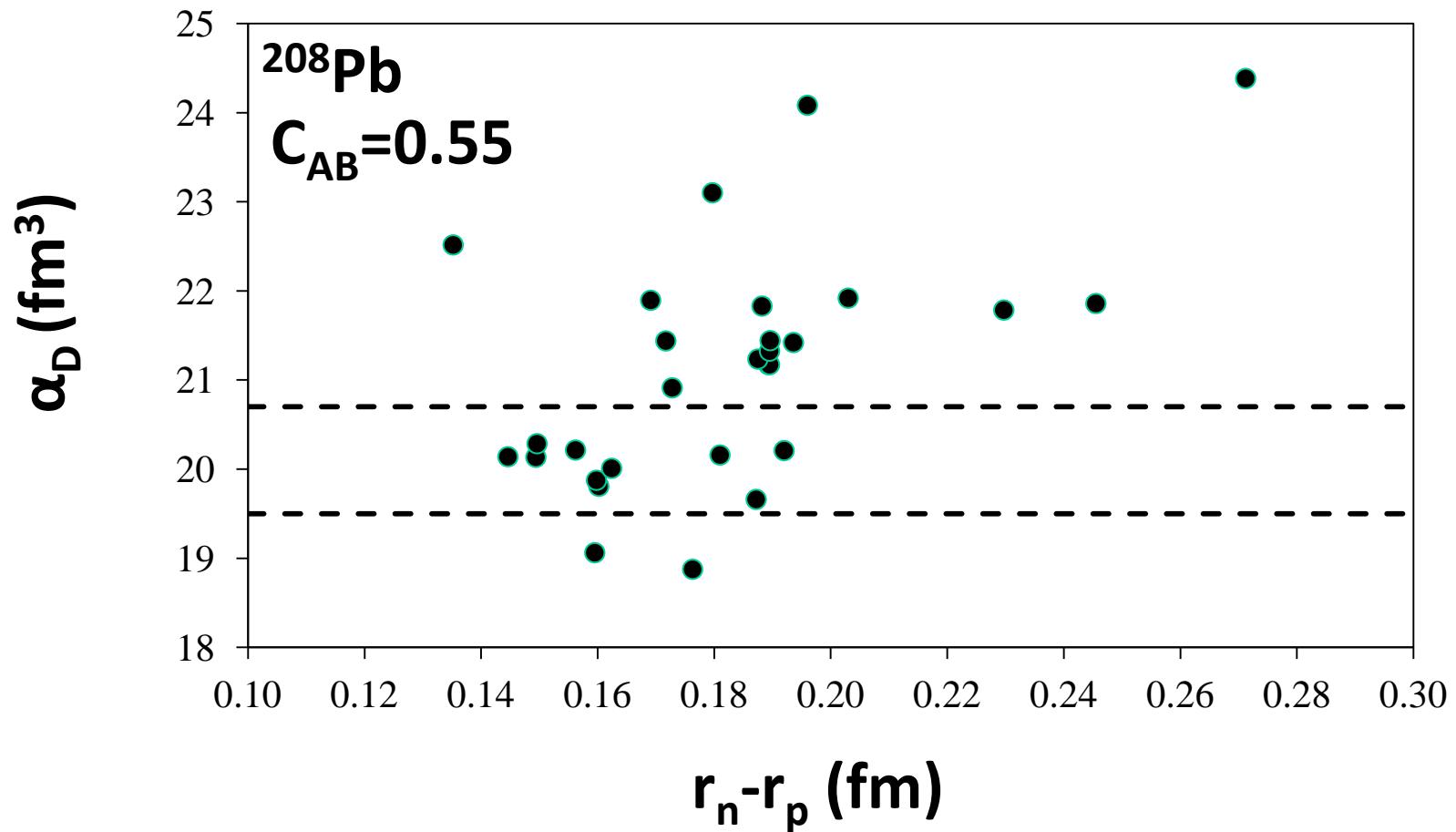
Fully self-consistent HF-RPA results for ISGMR centroid energy (in MeV) with the Skyrme interaction SK255, SGII and KDE0 are compared with the RRPA results using the NL3 interaction. Note the corresponding values of the nuclear matter incompressibility, K, and the symmetry energy , J, coefficients.  $\omega_1-\omega_2$  is the range of excitation energy. The experimental data are from TAMU.

Nucleus	$\omega_1-\omega_2$	Expt.	NL3	SK255	SGII	KDE0
$^{90}\text{Zr}$	0-60		18.7	18.9	17.9	18.0
	10-35	$17.81\pm 0.30$		18.9	17.9	18.0
$^{116}\text{Sn}$	0-60		17.1	17.3	16.4	16.6
	10-35	$15.85\pm 0.20$		17.3	16.4	16.6
$^{144}\text{Sm}$	0-60		16.1	16.2	15.3	15.5
	10-35	$15.40\pm 0.40$		16.2	15.2	15.5
$^{208}\text{Pb}$	0-60		14.2	14.3	13.6	13.8
	10-35	$13.96\pm 0.30$		14.4	13.6	13.8
K (MeV)			272	255	215	229
J (MeV)			37.4	37.4	26.8	33.0





Weak correlation with the symmetry energy,  $J$ .



# Conclusions

- We have developed a new EDFs based on Skyrme type interaction (KDE0, KDE, KDE0v1,... ) applicable to properties of rare nuclei and neutron stars.
- Fully self-consistent calculations of the compression modes (ISGMR and ISGDR) within HF-based RPA using Skyrme forces and within relativistic model lead a nuclear matter incompressibility coefficient of  $K_\infty = 240 \pm 20$  MeV, sensitivity to symmetry energy.
- Sensitivity to symmetry energy: IVGDR, GR in neutron rich nuclei,  $R_n - R_p$ , still open problems.
- Possible improvements:
  - Properly account for the isospin dependency of the spin-orbit interaction
  - Include additional data, such as IVGDR ( $J$ ) and ISGQR ( $m^*$ )

# Acknowledgments

**Work done at:**



**Work supported by:**



Grant number: PHY-0355200



Grant number: DOE-FG03-93ER40773